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Estimation of the Engineering Elastic Constants of a Directionally Solidified Superalloy for Finite Element Structural Analysis

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ESTIMATION OF THE ENGINEERING ELASTIC CONSTANTS OF A DIRECTIONALLY SOLIDIFIED SUPERALLOY FOR FINITE ELEMENT STRUCTURAL ANALYSIS

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SUMMARY

The temperature-dependent engineering elastic constants of a directionally solidified nickel-base superalloy were estimated from the single-crystal elastic constants of nickel and MAR-M002 superalloy by using Wells' method. In this method, the directionally solidified (columnar-grained) nickel-base superalloy was modeled as a transversely isotropic material, and the five independent elastic constants of the transversely isotropic material were determined from the three independent elastic constants of a cubic single crystal. Solidification for both the single crystals and the directionally solidified superalloy was assumed to be along the [001] direction. Temperature-dependent Young's moduli in longitudinal and transverse directions, shear moduli, and Poisson's ratios were tabulated for the directionally solidified nickel-base superalloy. These engineering elastic constants could be used as input for performing finite element structural analysis of directionally solidified turbine engine components.

INTRODUCTION

Development of gas-turbine engines has been hampered since conception by a lack of materials that can withstand high stress at elevated temperatures; however directionally solidified (DS) and single-crystal (SC) nickel-base superalloys that satisfy the durability requirements of turbine blades and vanes have now been developed. The DS nickel-base superalloys, which have been used in the construction of the first-stage high-pressure fuel turbopump blades of the space shuttle main engine (SSME), exhibit anisotropic mechanical behavior. This anisotropy of the material, the severe operating conditions (high temperatures, centrifugal loads etc.,) of the SSME, and the intricate geometry of the blades make the mechanical response of the turbine blades very complex. Finite element structural analyses are commonly used to study such mechanical response at elevated temperatures. In order to perform finite element analyses, the engineering elastic constants of the blade materials are required. In this report, temperature-dependent engineering elastic constants of a DS nickel-base superalloy are estimated by using the method proposed by Wells (ref. 1). The results are presented in tables and graphs.

BACKGROUND

Three independent elastic constants are required to define the elastic response of a cubic single crystal (ref. 2). These elastic constants can be expressed either as compliance coefficients (S_{11} , S_{12} , and S_{44}) or as stiffness coefficients (C_{11} , C_{12} , and C_{44}). The compliance coefficients are related to the stiffness coefficients by a unique set of equations (ref. 2).

The objective of this study was to use either set of these fundamental elastic constants of a cubic single crystal to estimate the engineering elastic constants of a DS nickel-base superalloy for performing finite element structural analyses. Such analyses are necessary to determine the stress-strain response of SSME components under thermal, mechanical, and aerodynamic loads. From the stress-strain responses, the fatigue lives of the SSME components can then be estimated.

In this work the primary orientation of both the SC and DS materials was assumed to be along the [001] crystal direction. In a DS superalloy, usually several grains with the same primary orientation are present in a columnar fashion as shown in figure 1; the secondary orientation for each of the columnar grains is random. Hence, a DS superalloy can be modeled as a transversely isotropic solid, provided a large number of grains are present in the material. Wells (ref. 1) reported a methodology for calculating the elastic constants of a DS nickel-base superalloy from the elastic constants of SC nickel. Wells' method was used to estimate the temperature-dependent engineering elastic constants of a DS nickel-base superalloy. The results, presented herein, are expected to be of particular interest to designers as well as structural analysts. In the following section, the analytical equations pertaining to the method proposed by Wells are presented.

ANALYTICAL PROCEDURE

Since the DS superalloy is assumed to be transversely isotropic, an axis of symmetry exists for this type of material (ref. 3). If the z -axis (fig. 1) is assumed to be the axis of symmetry, the strain-energy function W , according to Love (ref. 3), is given by

$$W = \frac{1}{2} \left[A(\epsilon_{xx}^2 + \epsilon_{yy}^2) + C\epsilon_{zz}^2 + 2F(\epsilon_{xx} + \epsilon_{yy})\epsilon_{zz} + 2(A - 2N)\epsilon_{xx}\epsilon_{yy} + L(\gamma_{yz}^2 + \gamma_{zx}^2) + N\gamma_{xy}^2 \right] \quad (1)$$

where ϵ_{xx} , ϵ_{yy} , and ϵ_{zz} and γ_{xy} , γ_{yz} , and γ_{zx} are the engineering normal and shear strains, respectively.¹ The material constants A , C , F , L , and N are the five independent constants that are required to characterize the elastic behavior of a transversely isotropic material.

The elastic stress-strain relationships for the DS material are as follows (ref. 1):

$$\sigma_{xx} = \frac{\partial W}{\partial \epsilon_{xx}} = A\epsilon_{xx} + F\epsilon_{zz} + (A - 2N)\epsilon_{yy} \quad (2)$$

$$\sigma_{yy} = \frac{\partial W}{\partial \epsilon_{yy}} = A\epsilon_{yy} + F\epsilon_{zz} + (A - 2N)\epsilon_{xx} \quad (3)$$

¹The symbols used by Wells (ref. 1) for engineering strains are different from those used by Love (ref. 3).

$$\sigma_{zz} = \frac{\partial W}{\partial \epsilon_{zz}} = C\epsilon_{zz} + F(\epsilon_{xx} + \epsilon_{yy}) \quad (4)$$

$$\tau_{xy} = \frac{\partial W}{\partial \gamma_{xy}} = N\gamma_{xy} \quad (5)$$

$$\tau_{yz} = \frac{\partial W}{\partial \gamma_{yz}} = L\gamma_{yz} \quad (6)$$

$$\tau_{zx} = \frac{\partial W}{\partial \gamma_{zx}} = L\gamma_{zx} \quad (7)$$

where σ_{xx} , σ_{yy} , and σ_{zz} and τ_{xy} , τ_{yz} , and τ_{zx} are the normal and shear components of stress, respectively.

Since primary orientations of both the single crystal and the DS nickel-base superalloy were assumed to be along the [001] direction (z-axis in fig. 1), compliance of the DS superalloy in the longitudinal direction is equal to the single-crystal compliance coefficient, S_{11} (ref. 1). In addition, for a single crystal oriented along the [001] direction, the ratio of transverse contraction to longitudinal extension along the [001] direction is isotropic and is equal to $-S_{12}/S_{11}$ (refs. 1 and 3).

Wells utilized the stress-strain relations (eqs. (2) to (7)) of a transversely isotropic material to derive the following relationships between the engineering elastic constants of a DS nickel-base superalloy and the elastic compliance coefficients (ref. 1)² of a single crystal:

$$E_L = E_z = \frac{\sigma_{zz}}{\epsilon_{zz}} = C - \frac{F^2}{(A - N)} = \frac{1}{S_{11}} \quad (8)$$

$$E_T = E_x = \frac{\sigma_{xx}}{\epsilon_{xx}} = \frac{4N(AC - NC - F^2)}{(AC - F^2)} = 2 \left[S_{11} (2S_{11} + S_{44} + 2S_{12}) \right]^{-1/2} \quad (9)$$

$$\nu_{zx} = - \frac{\epsilon_{xx}}{\epsilon_{zz}} = \frac{1}{2} \frac{F}{(A - N)} = - \frac{S_{12}}{S_{11}} \quad (10)$$

$$\nu_{yx} = - \frac{\epsilon_{xx}}{\epsilon_{yy}} = \frac{(F^2 - AC + 2NC)}{(F^2 - AC)} \quad (11)$$

$$G_{xy} = N = \left[2S_{44} (S_{11} - S_{12}) \right]^{-1/2} \quad (12)$$

²The definition of Poisson's ratio adopted in this paper is different from the definition used by Wells (ref. 1). In this paper, ν_{ij} refers to Poisson's ratio of the transverse strain in the j^{th} direction due to an imposed strain in the i^{th} direction. This definition is compatible with the commonly used definition for Poisson's ratio (ref. 4).

$$G_{yz} = L = \frac{1}{S_{44}} \quad (13)$$

where E_L and E_T are the longitudinal and transverse moduli of elasticity; G_{xy} and G_{yz} are the shear moduli; ν_{zx} and ν_{yx} are Poisson's ratios; and S_{11} , S_{12} , and S_{44} are the compliance coefficients of a cubic single crystal. Wells obtained the expressions for E_T (eq. (9)) and G_{xy} (eq. (12)) by averaging the respective values for all the possible secondary orientations in a cubic single crystal. Note that because of the symmetry of a transversely isotropic material, the following relationships exist between the different engineering elastic constants:

$$E_T = E_x = E_y \quad (14)$$

$$\nu_{zy} = \nu_{zx} \quad (15)$$

$$\nu_{xz} = \nu_{yz} \quad (16)$$

$$\nu_{xy} = \nu_{yx} \quad (17)$$

$$G_{xz} = G_{yz} = G_{zx} = G_{zy} \quad (18)$$

$$G_{xy} = G_{yx} \quad (19)$$

where E_i , G_{ij} , and ν_{ij} (for $i, j = x, y, z$ and $i \neq j$) are Young's moduli, shear moduli, and Poisson's ratios, respectively. For orthotropic materials, Poisson's ratios and Young's moduli are related by the following equation (ref. 4):

$$\frac{\nu_{ij}}{E_i} = \frac{\nu_{ji}}{E_j} ; \quad i, j = x, y, z \quad \text{and} \quad i \neq j \quad (20)$$

For a transversely isotropic material, which is a special case of an orthotropic material, equation (20) reduces to

$$\frac{\nu_{xz}}{E_x} = \frac{\nu_{zx}}{E_z} \quad (21)$$

The three independent elastic stiffness coefficients of a cubic single crystal are related to the elastic compliance coefficients by the following equations (ref. 2):

$$C_{11} = \frac{(S_{11} + S_{12})}{(S_{11} - S_{12})(S_{11} + 2S_{12})} \quad (22)$$

$$C_{12} = \frac{-S_{12}}{(S_{11} - S_{12})(S_{11} + 2S_{12})} \quad (23)$$

$$C_{44} = \frac{1}{S_{44}} \quad (24)$$

Alternatively, the elastic compliance coefficients of a single crystal can be expressed in terms of the elastic stiffness coefficients as

$$S_{11} = \frac{(C_{11} + C_{12})}{(C_{11} + 2C_{12})(C_{11} - C_{12})} \quad (25)$$

$$S_{12} = \frac{-C_{12}}{(C_{11} + 2C_{12})(C_{11} - C_{12})} \quad (26)$$

$$S_{44} = \frac{1}{C_{44}} \quad (27)$$

In order to obtain the engineering elastic constants of a DS superalloy from the elastic constants of a cubic single crystal, the five independent constants of the DS superalloy (A, C, F, L, and N in eqs. (8) to (13)) must be expressed in terms of the single-crystal compliance or stiffness coefficients. Constants L and N are already expressed in terms of the single-crystal compliance coefficients in equations (12) and (13), respectively. The others can be derived as follows: from equation (9)

$$\frac{(AC - NC - F^2)}{(AC - F^2)} = \frac{E_T}{4N} \quad (28)$$

Let

$$K = \frac{E_T}{4N} \quad (29)$$

By substituting for E_T and N from equations (9) and (12),

$$K = \sqrt{\frac{S_{44}(S_{11} - S_{12})}{2S_{11}(2S_{11} + S_{44} + 2S_{12})}} \quad (30)$$

Substituting equation (29) in (28) and rearranging the terms leads to

$$[(1 - K)A - N]C = (1 - K)F^2 \quad (31)$$

From equations (8) and (10), C and F can be expressed as

$$C = \frac{1}{S_{11}} + \frac{F^2}{(A - N)} \quad (32)$$

and

$$F = -2(A - N) \frac{S_{12}}{S_{11}} \quad (33)$$

Substituting equations (32) and (33) into equation (31), and solving for A yields

$$A = \frac{(NS_{11} - 4N^2KS_{12}^2)}{[(1 - K)S_{11} - 4NKS_{12}^2]} \quad (34)$$

Since N and K are already expressed in terms of the single-crystal compliance coefficients, with the preceding equations, A, F, and C can also be expressed in terms of the single-crystal compliance coefficients. Thus, all five independent DS superalloy elastic constants (A, C, F, L, and N) can be calculated from the single-crystal compliance coefficients. The engineering elastic constants for the DS superalloy can then be calculated from these five independent elastic constants.

RESULTS AND DISCUSSION

The temperature-dependent engineering elastic constants for a DS nickel-base superalloy were estimated from the SC nickel (ref. 5) and SC MAR-M002 (ref. 6) elastic constants available in the literature by applying the Wells method. Alers et al. (ref. 5) reported the temperature-dependent elastic stiffness coefficients for SC nickel. The following correlations were obtained for SC nickel by fitting second-degree polynomials in temperature to the reported values of C_{11} , C_{12} , and C_{44} :

$$C_{11} = 262.4 - 3.047 \times 10^{-2} T - 3.069 \times 10^{-5} T^2 \quad (35)$$

$$C_{12} = 150.7 - 2.631 \times 10^{-4} T - 6.692 \times 10^{-6} T^2 \quad (36)$$

$$C_{44} = 132.9 - 2.823 \times 10^{-2} T - 1.083 \times 10^{-5} T^2 \quad (37)$$

where stiffness coefficients C_{11} , C_{12} , and C_{44} are in gigapascals and temperature T is the absolute temperature in Kelvin. Figure 2 displays the data from reference 5 and the computed correlations for the stiffness coefficients. The compliance coefficients were calculated from the stiffness coefficients of the single crystal by using equations (25) to (27). The computed values of the five independent elastic constants of the DS material (A, C, F, L, and N as functions of temperature) are listed in table I. The temperature-dependent engineering elastic constants for DS nickel that were computed by using the equations described earlier are listed in table II. These engineering elastic constants are also shown in figures 3 and 4 (elastic and shear moduli as functions of temperature) and figure 5 (Poisson's ratios as functions of temperature).

Kuhn and Sockel (ref. 6) reported the temperature-dependent compliance coefficients for SC MAR-M002 (table III). Even though the data reported were

ranging from 25 to 1200 °C, there were not enough data points to permit curve-fitting. As a result, the five independent elastic constants of the DS material and the corresponding engineering elastic constants were calculated at each temperature. These constants are listed in tables IV and V, respectively.

The chemical compositions of SC MAR-M002 (ref. 6) and DS MAR-M246 (ref. 7) are shown in table VI. This table indicates that the chemical compositions of these two materials are similar. Huron (ref. 7) experimentally determined the longitudinal elastic modulus of DS MAR-M246 at several temperatures. In table VII these experimentally determined values are compared with the corresponding values estimated from SC nickel and SC MAR-M002.

In general, an estimation of the longitudinal modulus of DS MAR-M246 from SC MAR-M002 data is better than a similar estimation from the SC nickel data because the two alloys contain many of the same alloying elements, whereas SC nickel has no such alloying elements. Ideally, with the Wells method, elastic constants from SC MAR-M246 should have been used to determine the engineering elastic constants of DS MAR-M246. However, such single-crystal data were not readily available. No experimentally determined temperature-dependent transverse modulus, shear moduli, and Poisson's ratios were available for DS nickel-base superalloys to verify the accuracy of these engineering elastic constants.

The Wells method assumes that a sufficiently large number of columnar grains are present in the DS nickel-base superalloy. This assumption may not always be valid for engine components with small wall thicknesses. In such cases, the transverse elastic modulus E_T is not isotropic in nature. Thus, a DS nickel-base superalloy with relatively few grains in the transverse direction would deviate from the transversely isotropic material assumed in this study. Clearly then, the elastic constants determined in this study are applicable only when a large number of grains are present along the transverse direction in a DS nickel-base superalloy.

CONCLUDING REMARKS

The method proposed by Wells was used to predict the temperature-dependent engineering elastic constants of a directionally solidified (columnar-grained) nickel-base superalloy from single-crystal elastic constants of nickel and of MAR-M002 superalloy. In general, with Wells' method the elastic constants of any directionally solidified material can be determined from the elastic constants of a corresponding cubic single crystal. Scientists and structural analysts who work with commercial finite element codes will benefit the most from the results reported here since such codes require that material properties be input in the form of engineering elastic constants. The elastic constants obtained in this study can be used for performing finite element structural analysis on directionally solidified turbine engine components.

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TABLE I. - COMPUTED INDEPENDENT ELASTIC
CONSTANTS FOR DS NICKEL

Temperature, T, K	Independent elastic constants				
	A, GPa	C, GPa	F, GPa	L, GPa	N, GPa
0	274.8	252.9	137.6	132.9	86.1
50	272.8	251.1	137.4	131.4	85.0
100	270.5	249.1	137.2	129.9	83.9
150	268.1	247.0	136.8	128.4	82.7
200	265.4	244.7	136.4	126.8	81.4
250	262.6	242.2	136.0	125.1	80.1
300	259.5	239.5	135.4	123.4	78.7
350	256.5	236.7	134.8	121.6	77.2
400	252.8	233.6	134.1	119.8	75.7
450	249.1	230.3	133.3	118.0	74.1
500	245.2	226.8	132.4	116.0	72.5
550	241.1	223.1	131.4	114.0	70.7
600	236.7	219.2	130.3	112.0	68.9
650	232.0	215.0	129.1	109.9	67.1
700	227.1	210.6	127.7	107.8	65.1
750	221.8	205.9	126.2	105.6	63.1

TABLE II. - COMPUTED ENGINEERING ELASTIC CONSTANTS FOR DS NICKEL

Temperature, T, K	Young's moduli		Shear moduli		Poisson's ratios		
	E _z , GPa	E _x , GPa	G _{xz} , GPa	G _{xy} , GPa	ν _{xy}	ν _{zx}	ν _{xz}
0	152.4	196.0	132.9	86.1	0.138	0.365	0.469
50	150.4	193.7	131.4	85.0	.139	.366	.472
100	148.3	191.2	129.9	83.9	┌ └	.368	.474
150	145.9	188.5	128.4	82.7		.369	.477
200	143.5	185.6	126.8	81.4		.371	.480
250	140.9	182.6	125.1	80.1	.139	.373	.483
300	138.1	179.4	123.4	78.7	.139	.375	.487
350	135.1	176.0	121.6	77.2	.139	.377	.491
400	132.0	172.4	119.8	75.7	.138	.379	.495
450	128.7	168.7	118.0	74.1	.138	.381	.499
500	125.3	164.8	116.0	72.5	.136	.383	.504
550	121.7	160.6	114.0	70.7	.135	.386	.509
600	117.9	156.3	112.0	68.9	.133	.389	.515
650	113.9	151.8	109.9	67.1	.131	.391	.521
700	109.8	147.1	107.8	65.1	.129	.394	.528
750	105.5	142.2	105.6	63.1	.126	.398	.536

TABLE III. - COMPLIANCE COEFFICIENTS OF SC MAR-M002

[From ref. 6.]

Temperature T, K	Compliance coefficients, GPa ⁻¹		
	S ₁₁	S ₁₂	S ₄₄
298	0.007843	-0.003078	0.008000
873	.008960	-.003524	.009348
1073	.009671	-.003830	.010101
1173	.010288	-.004096	.010615
1273	.011198	-.004495	.011299
1373	.013071	-.005395	.012145
1473	.018115	-.007843	.013661

TABLE IV. - COMPUTED INDEPENDENT ELASTIC
CONSTANTS FOR DS MAR-M002

Temperature, T, K	Independent elastic constants				
	A, GPa	C, GPa	F, GPa	L, GPa	N, GPa
298	260.7	241.5	145.3	125.0	75.6
873	229.4	213.0	128.9	107.0	65.4
1073	215.6	200.6	122.8	99.0	60.5
1173	205.0	190.9	117.7	94.2	57.2
1273	191.6	178.5	111.2	88.5	53.0
1373	174.8	163.4	105.3	82.3	47.2
1473	141.9	133.5	90.4	73.2	37.5

TABLE V. - COMPUTED ENGINEERING ELASTIC CONSTANTS FOR DS MAR-M002

Temperature, T, K	Young's moduli		Shear moduli		Poisson's ratios		
	E _z , GPa	E _x , GPa	G _{xz} , GPa	G _{xy} , GPa	ν _{xy}	ν _{zx}	ν _{xz}
298	127.4	170.4	125.0	75.6	0.127	0.393	0.525
873	111.6	148.5	107.0	65.4	.135	.393	.524
1073	103.3	137.7	99.0	60.5	.138	.396	.528
1173	97.1	129.9	94.2	57.2	.136	.398	.533
1273	89.2	120.2	88.5	53.0	.132	.401	.541
1373	76.4	105.4	82.3	47.2	.117	.413	.569
1473	55.1	80.3	73.2	37.5	.070	.433	.630

TABLE VI. - CHEMICAL COMPOSITIONS OF SC MAR-M002 AND DS MAR-M246
[From refs. 6 and 7.]

Alloy	Composition, wt. %												
	C	Cr	Co	Ti	Al	W	Zr	B	Fe	Mo	Ta	Hf	Ni
Single crystal MAR-M002	0.15	9.00	10.00	1.20	5.50	10.00	0	0	<1.00	0	2.50	1.50	Balance
Directionally solidified MAR-M246	.16	8.13	10.15	1.59	5.60	9.35	.03	.018	.05	2.42	1.52	1.95	Balance

TABLE VII. - COMPARISON OF ESTIMATED AND OBSERVED LONGITUDINAL
ELASTIC MODULI OF DS MAR-M246

Temperature, T, K	Longitudinal elastic moduli				
	Experimentally observed, ^a GPa	Estimated from SC nickel		Estimated from SC MAR-M002	
		GPa	Percent error	GPa	Percent error
293	127.5	138.5	8.6	127.5	0
977	105.7	---	---	107.3	1.5
1200	91.6	---	---	95.0	3.7
1366	66.1	---	---	77.3	16.9

^aAverages of values reported in reference 7.

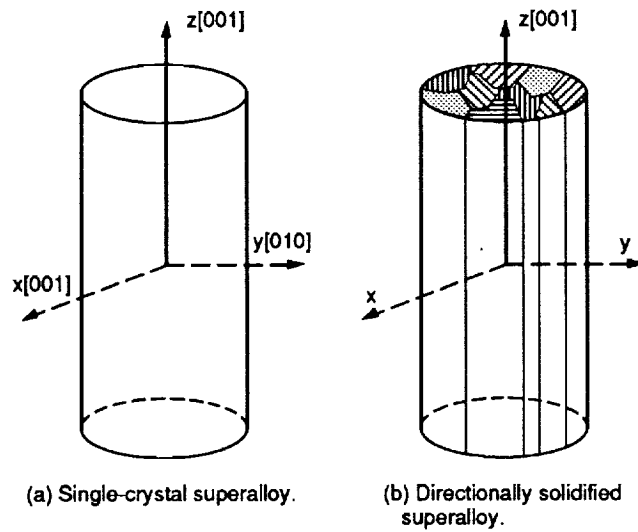


Figure 1.—Schematic of single-crystal and directionally solidified nickel-base superalloys.

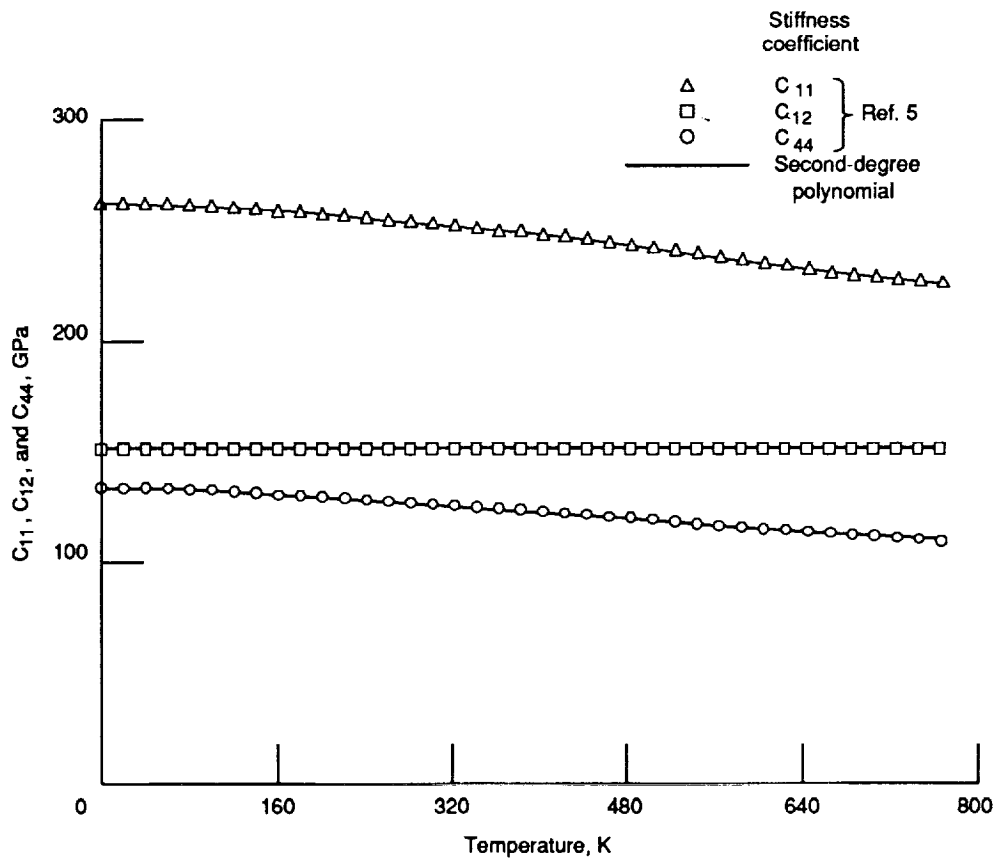


Figure 2.—Temperature-dependent stiffness coefficients for single-crystal nickel.

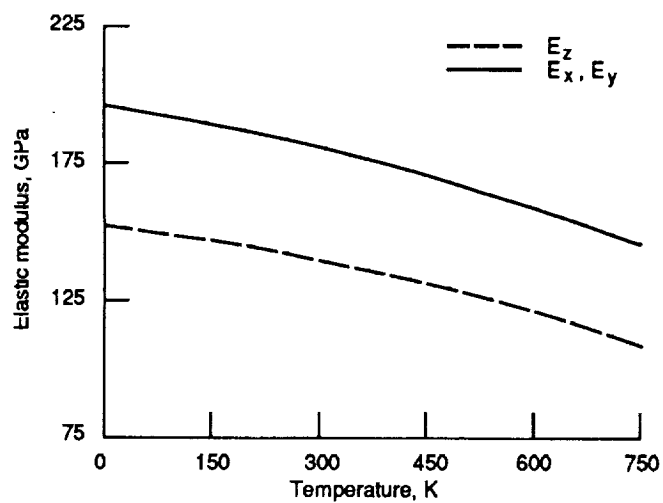


Figure 3.—Longitudinal (E_z) and transverse (E_x, E_y) Young's moduli of DS nickel.

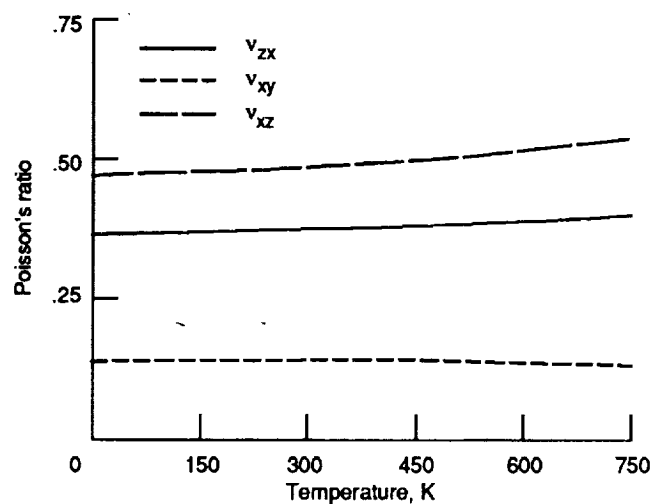


Figure 5.—Poisson's ratios of DS nickel.

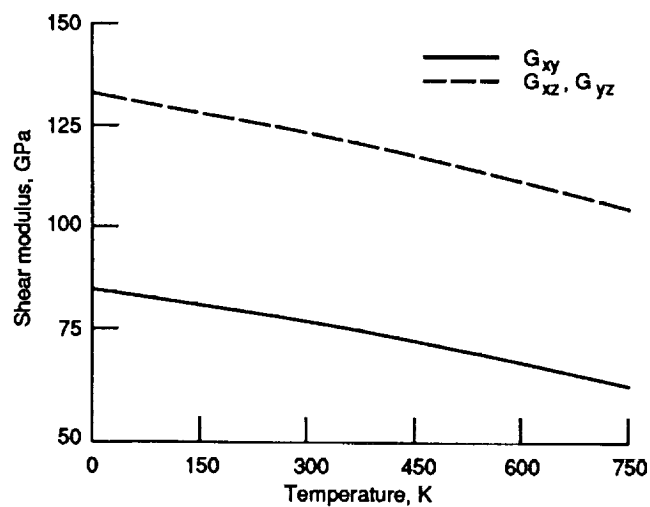


Figure 4.—Shear moduli of DS nickel.

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